

=> file casreact

FILE 'CASREACT' ENTERED AT 12:53:40 ON 24 SEP 2007

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FILE CONTENT:1840 - 22 Sep 2007 VOL 147 ISS 14

New CAS Information Use Policies, enter HELP USAGETERMS for details.

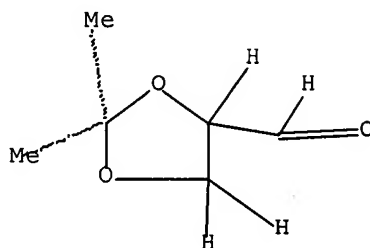
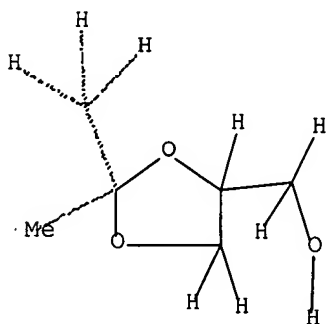
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*****
*
*      CASREACT now has more than 12 million reactions      *
*
*****
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

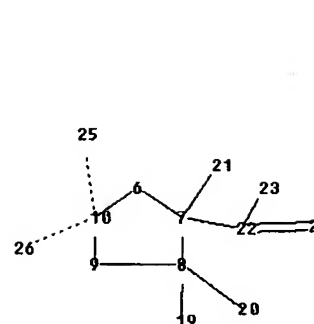
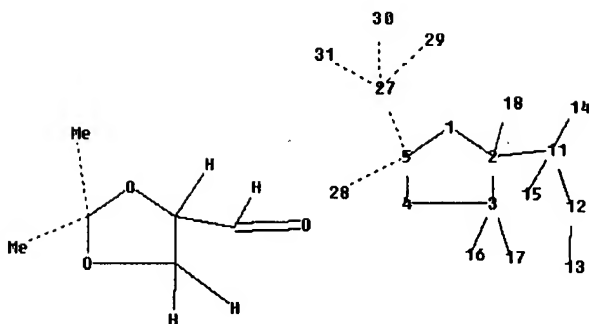
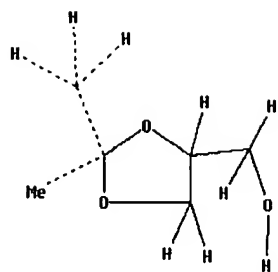
=> d stat que L12

L1 STR



Structure attributes must be viewed using STN Express query preparation:  
Uploading L1.str

10/576447



chain nodes :

11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

2-11 2-18 3-16 3-17 5-27 5-28 7-21 7-22 8-19 8-20 10-25 10-26 11-12

11-14 11-15 12-13 22-23 22-24 27-29 27-30 27-31

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 5-27 5-28 6-7 6-10 7-8 8-9 9-10 10-25 10-26 11-12

22-24 27-29 27-30 27-31

exact bonds :

2-11 2-18 3-16 3-17 7-21 7-22 8-19 8-20 11-14 11-15 12-13 22-23

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

19:CLASS 20:CLASS

21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS

29:CLASS 30:CLASS

31:CLASS

fragments assigned product role:

containing 6

fragments assigned reactant/reagent role:

containing 1

node mappings:

11:22

L3 10 SEA FILE=CASREACT SSS FUL L1 ( 11 REACTIONS)  
 L4 9 SEA FILE=CASREACT ABB=ON PLU=ON L3/COM  
 L8 1027 SEA FILE=CASREACT ABB=ON PLU=ON 2564-83-2  
 L9 128 SEA FILE=CASREACT ABB=ON PLU=ON 2226-96-2  
 L10 1 SEA FILE=CASREACT ABB=ON PLU=ON L4 (L) L8  
 L11 1 SEA FILE=CASREACT ABB=ON PLU=ON L4 (L) L9  
 L12 2 SEA FILE=CASREACT ABB=ON PLU=ON L10 OR L11

=> => file registry

FILE 'REGISTRY' ENTERED AT 13:13:51 ON 24 SEP 2007

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STRUCTURE FILE UPDATES: 23 SEP 2007 HIGHEST RN 947726-74-1  
 DICTIONARY FILE UPDATES: 23 SEP 2007 HIGHEST RN 947726-74-1

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> file zcaplus

FILE 'ZCAPLUS' ENTERED AT 13:13:54 ON 24 SEP 2007  
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FILE COVERS 1907 - 24 Sep 2007 VOL 147 ISS 14  
 FILE LAST UPDATED: 23 Sep 2007 (20070923/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L35

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L5      26 SEA FILE=REGISTRY ABB=ON  PLU=ON  (100-79-8/RN OR 5736-03-8/RN
        OR 75-09-2/RN OR 121-44-8/RN OR 14347-78-5/RN OR 22323-80-4/RN
        OR 2564-83-2/RN OR 26299-14-9/RN OR 67-68-5/RN OR 7732-18-5/RN
        OR 79-37-8/RN OR 87-90-1/RN OR 110-86-1/RN OR 127-09-3/RN OR
        1333-82-0/RN OR 1344-28-1/RN OR 144-55-8/RN OR 20667-12-3/RN
        OR 2226-96-2/RN OR 397863-03-5/RN OR 67-64-1/RN OR 75-05-8/RN
        OR 7647-01-0/RN OR 7647-15-6/RN OR 7664-93-9/RN OR 7681-52-9/RN
        )
L6      4 SEA FILE=REGISTRY ABB=ON  PLU=ON  NC5/ESS AND L5
L7      2 SEA FILE=REGISTRY ABB=ON  PLU=ON  L6 AND C>8
L14     5363 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L7
L15     5 SEA FILE=REGISTRY ABB=ON  PLU=ON  L5 AND OCOC2/ES
```

10/576447

L16 2139 SEA FILE=ZCAPLUS ABB=ON PLU=ON L15  
L17 3 SEA FILE=ZCAPLUS ABB=ON PLU=ON L14 AND L16  
L19 1 SEA FILE=REGISTRY ABB=ON PLU=ON "1,3-DIOXOLANE-4-CARBOXALDEHY  
DE, 2,2-DIMETHYL-, (4S) -"/CN  
L20 1 SEA FILE=REGISTRY ABB=ON PLU=ON "1,3-DIOXOLANE-4-CARBOXALDEHY  
DE, 2,2-DIMETHYL-, (4R) -"/CN  
L21 1 SEA FILE=REGISTRY ABB=ON PLU=ON "1,3-DIOXOLANE-4-CARBOXALDEHY  
DE, 2,2-DIMETHYL-"/CN  
L22 1317 SEA FILE=ZCAPLUS ABB=ON PLU=ON (L19 OR L20 OR L21)  
L23 4 SEA FILE=ZCAPLUS ABB=ON PLU=ON L22 AND L7  
L25 1 SEA FILE=REGISTRY ABB=ON PLU=ON 1,3-DIOXOLANE-4-METHANOL,  
2,2-DIMETHYL-/CN  
L26 2 SEA FILE=REGISTRY ABB=ON PLU=ON ("1,3-DIOXOLANE-4-METHANOL,  
2,2-DIMETHYL-, (4R) -"/CN OR "1,3-DIOXOLANE-4-METHANOL,  
2,2-DIMETHYL-, (4S) -"/CN)  
L27 3 SEA FILE=REGISTRY ABB=ON PLU=ON L25 OR L26  
L28 1317 SEA FILE=ZCAPLUS ABB=ON PLU=ON (L19 OR L20 OR L21)  
L29 2192 SEA FILE=ZCAPLUS ABB=ON PLU=ON L27  
L30 5363 SEA FILE=ZCAPLUS ABB=ON PLU=ON L7  
L31 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON L28 AND L29 AND L30  
L32 4 SEA FILE=ZCAPLUS ABB=ON PLU=ON L17 OR L23 OR L31  
L33 4 SEA FILE=ZCAPLUS ABB=ON PLU=ON L28 AND L30  
L34 3 SEA FILE=ZCAPLUS ABB=ON PLU=ON L29 AND L30  
L35 5 SEA FILE=ZCAPLUS ABB=ON PLU=ON (L32 OR L33 OR L34)

=> dup rem L12 L35

FILE 'CASREACT' ENTERED AT 13:14:14 ON 24 SEP 2007  
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PROCESSING COMPLETED FOR L12  
PROCESSING COMPLETED FOR L35

L36 5 DUP REM L12 L35 (2 DUPLICATES REMOVED)  
ANSWERS '1-2' FROM FILE CASREACT  
ANSWERS '3-5' FROM FILE ZCAPLUS

=> d ibib abs hit L36 1-2; d ibib abs hitstr L36 3-5

L36 ANSWER 1 OF 5 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 1  
ACCESSION NUMBER: 142:430492 CASREACT Full-text  
TITLE: Process for the preparation of glyceraldehyde  
acetone from solketal via oxidation reaction  
INVENTOR(S): Quaedflieg, Peter Jan Leonard Mario; Alsters, Paulus  
Lambertus; Pojarliev, Peter; Jary, Walther Gunther  
PATENT ASSIGNEE(S): DSM IP Assets B.V., Neth.  
SOURCE: PCT Int. Appl., 27 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005040149 A1 20050506 WO 2004-EP12064 20041025

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2543303 A1 20050506 CA 2004-2543303 20041025

EP 1678158 A1 20060712 EP 2004-817268 20041025

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

CN 1875014 A 20061206 CN 2004-80031932 20041025

JP 2007522097 T 20070809 JP 2006-537158 20041025

IN 2006DN02387 A 20070803 IN 2006-DN2387 20060428

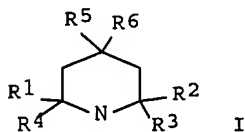
US 2007129553 A1 20070607 US 2006-576447 20060714

PRIORITY APPLN. INFO.: EP 2003-78392 20031028

WO 2004-EP12064 20041025

OTHER SOURCE(S): MARPAT 142:430492

GI

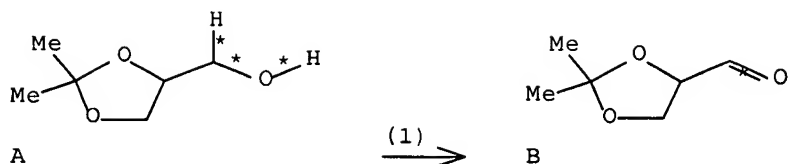


AB The invention relates to a process for the preparation of glyceraldehyde acetonide I, wherein R1-R4 are independently alkyl with 1 to 6 C-atoms and wherein R5 and R6 either both stand for H or an alkoxy group with 1 to 6 C-atoms or one stands for H and the other stands for an alkoxy group with 1 to 6 C-atoms, an alkylcarbonyloxy group with 1 to 6 C-atoms, an arylcarbonyloxy group with the carbonyloxy group having 1 to 6 C-atoms or an alkylcarbonylamino group with 1 to 6 C-atoms; or wherein R5 and R6 together stand for ketal groups, by oxidation of 2,2-dimethyl-1,3-dioxolane-4- methanol by an oxidizing agent, wherein the 2,2-dimethyl-1,3-dioxolane-4- methanol is oxidized by an organic N-chloro compound in the presence of an inert base and TEMPO or a TEMPO-derivative. In one embodiment of the invention enantiomerically enriched glyceraldehyde acetonide is prepared from the corresponding enantiomerically enriched 2,2-dimethyl-1,3-dioxolane-4- methanol. Preferably, the organic N-chloro compound is trichloroisocyanuric acid or dichlorodimethyl hydantoin. Preferably, the inert base is sodium acetate or sodium bicarbonate. Thus, oxidation of (R)-solketal with trichloroisocyanuric acid in presence of TEMPO in acetone gave (S)-glyceraldehyde acetonide in 80% yield.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

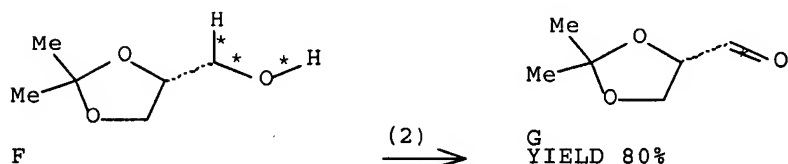
RX(1) OF 4 A ==> B

10/576447



RX(1)      RCT    A 100-79-8  
              RGT    C 87-90-1 Isocyanuric chloride  
              PRO    B 5736-03-8  
              CAT    2564-83-2 Me4-piperidoxyl  
              SOL    75-05-8 MeCN  
              CON    30 minutes, room temperature  
              NTE    optimization study, optimized on catalyst and oxidant

RX(2) OF 4      F ==> G...



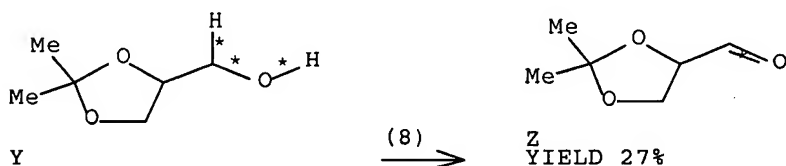
RX(2)      RCT    F 14347-78-5  
              RGT    C 87-90-1 Isocyanuric chloride, H 127-09-3 AcONa  
              PRO    G 22323-80-4  
              CAT    2564-83-2 Me4-piperidoxyl  
              SOL    67-64-1 Me2CO  
              CON    SUBSTAGE(1) 25 deg C  
                      SUBSTAGE(2) 8 minutes, 25 deg C -> 59 deg C  
                      SUBSTAGE(3) 30 minutes  
              NTE    optimization study, stereoselective

L36 ANSWER 2 OF 5 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 2  
 ACCESSION NUMBER:      143:349015 CASREACT Full-text  
 TITLE:                      Technical Production of Aldehydes by Continuous Bleach  
                                  Oxidation of Alcohols Catalyzed by 4-Hydroxy-TEMPO  
 AUTHOR(S):                Fritz-Langhals, Elke  
 CORPORATE SOURCE:       Consortium fuer Elektrochemische Industrie GmbH,  
                                  Wacker-Chemie GmbH, Munich, D-81379, Germany  
 SOURCE:                    Organic Process Research & Development (2005), 9(5),  
                                  577-582  
                                  CODEN: OPRDFK; ISSN: 1083-6160  
 PUBLISHER:                American Chemical Society  
 DOCUMENT TYPE:           Journal  
 LANGUAGE:                English

AB Aldehydes were easily prepared from the corresponding alcs. in good to excellent yields by oxidation with tech. bleach and catalytic amts. of 4-hydroxy-2,2,6,6-tetramethyl-piperidine-1-oxyl (4-hydroxy TEMPO, HOT). Whereas the well-known batch process performed on laboratory scale is not suitable for the tech. synthesis especially of activated  $\beta$ -substituted aldehydes, this transformation can be performed continuously in a simple tube reactor. This layout meets all requirements necessary for the process, i.e., turbulent mixing of the biphasic mixture, removal of heat, short contact times, and high output. Thus, a single tube of 3 mm diameter renders about 60 mol of aldehyde per day.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(8) OF 15 Y ==> Z



RX(8) RCT Y 100-79-8

STAGE(1)

RGT L 144-55-8 NaHCO<sub>3</sub>  
 CAT 2226-96-2 1-Piperidinyloxy, 4-hydroxy-2,2,6,6-tetramethyl-, 7647-15-6 NaBr  
 SOL 7732-18-5 Water, 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON 10 seconds, -10 deg C

STAGE(2)

RGT C 7681-52-9 NaOCl, D 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
 SOL 7732-18-5 Water  
 CON 3 minutes, pH 9.5

PRO Z 5736-03-8

L36 ANSWER 3 OF 5 ZCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2006:538331 ZCAPLUS Full-text  
 DOCUMENT NUMBER: 145:27400  
 TITLE: Novel method for the preparation of aldehydes or ketones by TEMPO-catalyzed oxidation of primary or secondary alcohols  
 INVENTOR(S): Igi, Kimitaka; Hirata, Makoto; Mikami, Masafumi  
 PATENT ASSIGNEE(S): Daiso Co., Ltd., Japan  
 SOURCE: U.S. Pat. Appl. Publ., 5 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006122434	A1	20060608	US 2005-290474	20051201
US 7208634	B2	20070424		
JP 2006182764	A	20060713	JP 2005-339162	20051124
EP 1666441	A1	20060607	EP 2005-257406	20051201

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU

PRIORITY APPLN. INFO.:

JP 2004-350780

A 20041203

OTHER SOURCE(S):

CASREACT 145:27400; MARPAT 145:27400

AB A method for preparing an aldehyde or ketone by oxidizing a primary or secondary alc. with a N-bromoamide compound or a combination of a N-chlorosuccinimide and a compound having bromide ion in the presence of a nitroxyl radical compound R0R1R2C-N(O)-CR0R3R4 [wherein R0 - R4 = alkyl; two R0 may link together to form a 5 to 7 membered ring with the nitrogen atom] is disclosed. For example, to a cooled suspension of 1-octanol (2.0 g), sodium bicarbonate (1.6 g) and TEMPO (24 mg) in dichloromethane (15 mL) was added NBS (3.0 g) in three portions at an ice bath. Usual workup and distillation gave 1-octanal in 88% yield. Alternatively, this reaction was carried out in the presence of catalytic amount of NaBr using 4-hydroxy TEMPO and NCS instead of TEMPO and NBS to afford 1-octanal in 85% yield.

IT 2226-96-2, 4-Hydroxy TEMPO 2564-83-2, TEMPO

RL: CAT (Catalyst use); USES (Uses)

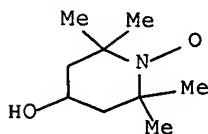
(catalyst; preparation of aldehydes or ketones by TEMPO-catalyzed oxidation

of

primary or secondary alcs. with N-bromoamides or a combination of N-chlorosuccinimide and bromides)

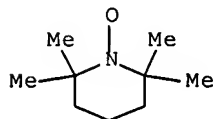
RN 2226-96-2 ZCAPLUS

CN 1-Piperidinyloxy, 4-hydroxy-2,2,6,6-tetramethyl- (CA INDEX NAME)



RN 2564-83-2 ZCAPLUS

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl- (CA INDEX NAME)



IT 22323-80-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of aldehydes or ketones by TEMPO-catalyzed oxidation of



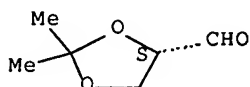
primary or

secondary alcs. with N-bromoamides or a combination of  
N-chlorosuccinimide and bromides)

RN 22323-80-4 ZCAPLUS

CN 1,3-Dioxolane-4-carboxaldehyde, 2,2-dimethyl-, (4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 4 OF 5 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:562365 ZCAPLUS Full-text

DOCUMENT NUMBER: 145:62870

TITLE: Process for preparing  $\alpha,\beta$ -unsaturated  
carboxylate esters

INVENTOR(S): Igi, Kimitaka; Hirata, Makoto; Mikami, Masafumi;  
Nagano, Yoshifumi

PATENT ASSIGNEE(S): Daiso Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 11 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

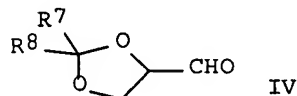
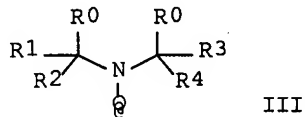
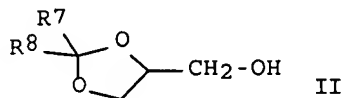
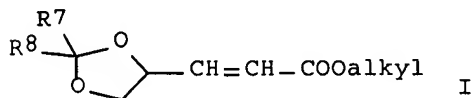
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1669353	A1	20060614	EP 2005-257405	20051201
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
JP 2006182763	A	20060713	JP 2005-339144	20051124
PRIORITY APPLN. INFO.:			JP 2004-350777	A 20041203
OTHER SOURCE(S):	CASREACT 145:62870; MARPAT 145:62870			

GI



AB A process for preparing an  $\alpha,\beta$ -unsatd. ester [I; R7, R8 = H, C1-6 alkyl, Ph; e.g., (S)-3-(2,2-dimethyl-1,3-dioxolan-4-yl)-2-propenoic acid Me ester] comprises oxidizing a glycerol acetal derivative [II; e.g., (S)-glycerol acetone] in the presence of a nitroxyl radical compound [III; R0-R4 = (un)branched alkyl; R0R0 = may form a ring; e.g., TEMPO] and a co-oxidant (e.g., diacetoxyiodobenzene) to prepare a glyceraldehyde (IV) and then reacting it with a phosphonoacetic acid alkyl ester (e.g., phosphonoacetic acid tri-Me ester) or a (triphenylphosphoranylidene)acetic acid alkyl ester to give I.

IT 22323-82-6

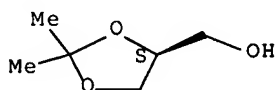
RL: RCT (Reactant); RACT (Reactant or reagent)

(in a process for preparing  $\alpha,\beta$ -unsatd. carboxylate esters)

RN 22323-82-6 ZCAPLUS

CN 1,3-Dioxolane-4-methanol, 2,2-dimethyl-, (4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



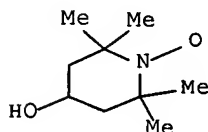
IT 2226-96-2 2564-83-2, TEMPO

RL: RGT (Reagent); RACT (Reactant or reagent)

(in a process for preparing  $\alpha,\beta$ -unsatd. carboxylate esters)

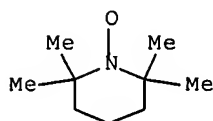
RN 2226-96-2 ZCAPLUS

CN 1-Piperidinyloxy, 4-hydroxy-2,2,6,6-tetramethyl- (CA INDEX NAME)



RN 2564-83-2 ZCAPLUS

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl- (CA INDEX NAME)



REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 5 OF 5 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:719185 ZCAPLUS Full-text

DOCUMENT NUMBER: 139:7143

TITLE: A  $\beta$ -lactam route to short peptide segments related to angiotensin-converting enzyme (ACE) inhibitors

AUTHOR(S): Palomo, Claudio; Ganboa, Inaki; Oiarbide, Mikel; Sciano, Giuseppe Tomasi; Miranda, Jose I.

CORPORATE SOURCE: Dep. de Quim. Organica, Fac. de Quim., Univ. del Pais Vasco, San Sebastian, 20080, Spain

SOURCE: ARKIVOC (Gainesville, FL, United States) [online computer file] (2002), (5), 8-16  
CODEN: AGFUAR  
URL: <http://www.arkat-usa.org/ark/journal/2002/MManas/MM-334C/MM-334C.pdf>

PUBLISHER: Arkat USA Inc.

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

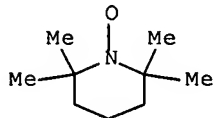
OTHER SOURCE(S): CASREACT 139:7143

AB The stereocontrolled synthesis of the Angiotensin Converting Enzyme (ACE) inhibitor enalapril is reported. The key transformation of the synthesis is a formal carboxylation of imines, which lies in the sequence: imine-ketene [2+2] cycloaddn. reaction, ring expansion of the resulting 3-hydroxy  $\beta$ -lactam to a N-carboxy  $\alpha$ -amino acid anhydride (NCA), and final opening of the NCA with alcs.

IT 2564-83-2  
RL: CAT (Catalyst use); USES (Uses)  
(stereocontrolled synthesis of enalapril via  $\beta$ -lactam route)

RN 2564-83-2 ZCAPLUS

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl- (CA INDEX NAME)

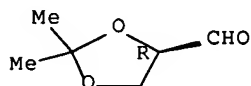


IT 15186-48-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(stereocontrolled synthesis of enalapril via  $\beta$ -lactam route)

RN 15186-48-8 ZCAPLUS

CN 1,3-Dioxolane-4-carboxaldehyde, 2,2-dimethyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his full

(FILE 'HOME' ENTERED AT 12:46:02 ON 24 SEP 2007)

FILE 'CASREACT' ENTERED AT 12:46:10 ON 24 SEP 2007

L1 STRUCTURE UPLOADED  
 L2 2 SEA SSS SAM L1 ( 2 REACTIONS)  
 D SCA  
 L3 10 SEA SSS FUL L1 ( 11 REACTIONS)  
 L4 9 SEA ABB=ON PLU=ON L3/COM  
 D SCA  
 SAVE TEMP CHANDRL1/A L3  
 SEL L4 RX

FILE 'REGISTRY' ENTERED AT 12:49:59 ON 24 SEP 2007

L5 26 SEA ABB=ON PLU=ON (100-79-8/RN OR 5736-03-8/RN OR 75-09-2/RN  
 OR 121-44-8/RN OR 14347-78-5/RN OR 22323-80-4/RN OR 2564-83-2/R  
 N OR 26299-14-9/RN OR 67-68-5/RN OR 7732-18-5/RN OR 79-37-8/RN  
 OR 87-90-1/RN OR 110-86-1/RN OR 127-09-3/RN OR 1333-82-0/RN OR  
 1344-28-1/RN OR 144-55-8/RN OR 20667-12-3/RN OR 2226-96-2/RN  
 OR 397863-03-5/RN OR 67-64-1/RN OR 75-05-8/RN OR 7647-01-0/RN  
 OR 7647-15-6/RN OR 7664-93-9/RN OR 7681-52-9/RN)  
 L6 4 SEA ABB=ON PLU=ON NC5/ESS AND L5  
 D SCA  
 L7 2 SEA ABB=ON PLU=ON L6 AND C>8  
 D RN 1-2

FILE 'CASREACT' ENTERED AT 12:52:11 ON 24 SEP 2007

L8 1027 SEA ABB=ON PLU=ON 2564-83-2  
 L9 128 SEA ABB=ON PLU=ON 2226-96-2  
 L10 1 SEA ABB=ON PLU=ON L4 (L) L8  
 L11 1 SEA ABB=ON PLU=ON L4 (L) L9  
 L12 2 SEA ABB=ON PLU=ON L10 OR L11  
 D SCA

FILE 'CASREACT' ENTERED AT 12:53:40 ON 24 SEP 2007

D STAT QUE L12  
 D IBIB ABS HIT L12 1-2

FILE 'STNGUIDE' ENTERED AT 12:59:05 ON 24 SEP 2007

FILE 'REGISTRY' ENTERED AT 13:01:38 ON 24 SEP 2007

L13 144050 SEA ABB=ON PLU=ON OCOC2/ES

FILE 'ZCAPLUS' ENTERED AT 13:01:55 ON 24 SEP 2007

L14 5363 SEA ABB=ON PLU=ON L7

FILE 'REGISTRY' ENTERED AT 13:02:51 ON 24 SEP 2007

L15 5 SEA ABB=ON PLU=ON L5 AND OCOC2/ES

FILE 'ZCAPLUS' ENTERED AT 13:03:14 ON 24 SEP 2007

L16 2139 SEA ABB=ON PLU=ON L15  
 L17 3 SEA ABB=ON PLU=ON L14 AND L16  
 D SCA

FILE 'CASREACT, ZCAPLUS' ENTERED AT 13:06:09 ON 24 SEP 2007

L18 3 DUP REM L12 L17 (2 DUPLICATES REMOVED)  
 ANSWERS '1-2' FROM FILE CASREACT

10/576447

ANSWER '3' FROM FILE ZCAPLUS  
D IBIB ABS HITSTR L18 3

FILE 'REGISTRY' ENTERED AT 13:08:44 ON 24 SEP 2007

E "1,3-DIOXOLANE-4-CARBOXALDEHYDE, 2,2-DIMETHYL-, (4S)-"/CN  
L19 1 SEA ABB=ON PLU=ON "1,3-DIOXOLANE-4-CARBOXALDEHYDE, 2,2-DIMETH  
YL-, (4S)-"/CN  
L20 1 SEA ABB=ON PLU=ON "1,3-DIOXOLANE-4-CARBOXALDEHYDE, 2,2-DIMETH  
YL-, (4R)-"/CN  
L21 1 SEA ABB=ON PLU=ON "1,3-DIOXOLANE-4-CARBOXALDEHYDE, 2,2-DIMETH  
YL-"/CN  
E "1,3-DIOXOLANE-4-CARBOXALDEHYDE, 2,2-DIMETHYL-"/CN

FILE 'ZCAPLUS' ENTERED AT 13:09:59 ON 24 SEP 2007

L22 1317 SEA ABB=ON PLU=ON (L19 OR L20 OR L21)  
L23 4 SEA ABB=ON PLU=ON L22 AND L7

FILE 'REGISTRY' ENTERED AT 13:10:41 ON 24 SEP 2007

L24 3 SEA ABB=ON PLU=ON (L19 OR L20 OR L21)  
D SCA  
D SCA L15  
E 1,3-DIOXOLANE-4-METHANOL, 2,2-DIMETHYL-, /CN  
E 1,3-DIOXOLANE-4-METHANOL, 2,2-DIMETHYL-/CN  
L25 1 SEA ABB=ON PLU=ON 1,3-DIOXOLANE-4-METHANOL, 2,2-DIMETHYL-/CN  
L26 2 SEA ABB=ON PLU=ON ("1,3-DIOXOLANE-4-METHANOL, 2,2-DIMETHYL-,  
(4R)-"/CN OR "1,3-DIOXOLANE-4-METHANOL, 2,2-DIMETHYL-,  
(4S)-"/CN)  
L27 3 SEA ABB=ON PLU=ON L25 OR L26

FILE 'ZCAPLUS' ENTERED AT 13:12:18 ON 24 SEP 2007

L28 1317 SEA ABB=ON PLU=ON (L19 OR L20 OR L21)  
L29 2192 SEA ABB=ON PLU=ON L27  
L30 5363 SEA ABB=ON PLU=ON L7  
L31 2 SEA ABB=ON PLU=ON L28 AND L29 AND L30  
L32 4 SEA ABB=ON PLU=ON L17 OR L23 OR L31  
L33 4 SEA ABB=ON PLU=ON L28 AND L30  
L34 3 SEA ABB=ON PLU=ON L29 AND L30  
L35 5 SEA ABB=ON PLU=ON (L32 OR L33 OR L34)

FILE 'REGISTRY' ENTERED AT 13:13:51 ON 24 SEP 2007

FILE 'ZCAPLUS' ENTERED AT 13:13:54 ON 24 SEP 2007  
D STAT QUE L35

FILE 'CASREACT, ZCAPLUS' ENTERED AT 13:14:14 ON 24 SEP 2007

L36 5 DUP REM L12 L35 (2 DUPLICATES REMOVED)  
ANSWERS '1-2' FROM FILE CASREACT  
ANSWERS '3-5' FROM FILE ZCAPLUS  
D IBIB ABS HIT L36 1-2  
D IBIB ABS HITSTR L36 3-5

FILE HOME

FILE CASREACT

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FILE CONTENT:1840 - 22 Sep 2007 VOL 147 ISS 14

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*
*      CASREACT now has more than 12 million reactions
*
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This file contains CAS Registry Numbers for easy and accurate substance identification.

#### FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 SEP 2007 HIGHEST RN 947726-74-1  
DICTIONARY FILE UPDATES: 23 SEP 2007 HIGHEST RN 947726-74-1

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<http://www.cas.org/support/stngen/stndoc/properties.html>

#### FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Sep 21, 2007 (20070921/UP).

#### FILE ZCAPLUS

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FILE COVERS 1907 - 24 Sep 2007 VOL 147 ISS 14  
FILE LAST UPDATED: 23 Sep 2007 (20070923/ED)

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10/576447

This file contains CAS Registry Numbers for easy and accurate  
substance identification.

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